

STN 1-17-03  
Author Search

L3 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS  
AN 1998:142921 CAPLUS  
TI Olefin trimerization with 1,3,5-triazacyclohexane complexes of chromium  
AU Koehn, R. D.; Haufe, M.; Kociok-Koehn, G.  
CS Institut f. Anorg. u. Analyt. Chemie, TU Berlin, Berlin, 10623, Germany  
SO Book of Abstracts, 215th ACS National Meeting, Dallas, March 29-April 2  
(1998), INOR-278 Publisher: American Chemical Society, Washington, D. C.  
CODEN: 65QTAA  
DT Conference; Meeting Abstract  
LA English  
AB Most catalytic olefin oligomerizations or polymers. proceed via the hydride mechanism. An exception appears to be the selective trimerization of ethylene to 1-hexene with chromium catalysts- a reaction that may soon be an industrial process. However, the mechanism of this important transformation is still largely unclear. Jolly could support a possible mechanism with oxidative addn. of two olefins to a chromium complex giving a metallacyclopentane which inserts a third ethylene to give a metallacycloheptane before .beta.-hydride and reductive elimination regenerates the original complex and 1-hexene. We have found that N-substituted triazacyclohexane complexes of CrCl<sub>3</sub> react with MAO to give a homogeneous catalyst for the selective trimerization of alpha-olefins. This allows the detailed study of the mechanism by observation of the reaction in the NMR or UV/Vis and by introducing olefinic N-substituents that participate in the initiation and trimerization.

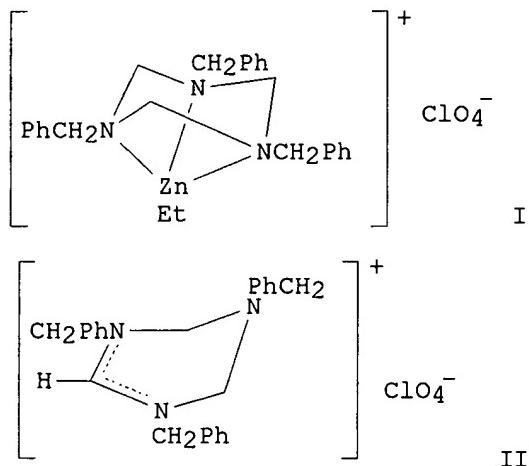
L3 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS  
AN 1997:784429 CAPLUS  
DN 127:354654  
TI The Chemistry of 1,3,5-Triazacyclohexane Complexes. 7. Synthesis and Characterization of the Cobalt(II) Methoxide Core {Co<sub>3</sub>(OMe)<sub>4</sub>}<sup>2+</sup>  
AU Koehn, Randolph D.; Haufe, Matthias; Kociok-Koehn,  
Gabriele; Filippou, Alexander C.  
CS Institut fuer Anorganische und Analytische Chemie, Technische Universitaet Berlin, Berlin, D-10623, Germany  
SO Inorganic Chemistry (1997), 36(26), 6064-6069  
CODEN: INOCAJ; ISSN: 0020-1669  
PB American Chemical Society  
DT Journal  
LA English  
CC 78-7 (Inorganic Chemicals and Reactions)  
Section cross-reference(s): 75  
AB The authors report the synthesis and characterization of the 1st .eta.3-1,3,5-trimethyl-1,3,5-triazacyclohexane, (Me<sub>3</sub>TAC) alkoxo complexes. Dehydration of [Co(H<sub>2</sub>O)<sub>6</sub>]<sup>2+</sup> with 2,2-dimethoxypropane or HC(OMe)<sub>3</sub> and subsequent treatment with Me<sub>3</sub>TAC gave the methoxo cube fragment clusters [{(Me<sub>3</sub>TAC)Co}<sub>3</sub>(OMe)<sub>4</sub>}(X)<sub>2</sub> (X = B(C<sub>6</sub>F<sub>5</sub>)<sub>4</sub> (2a) and B(m-C<sub>6</sub>H<sub>3</sub>(CF<sub>3</sub>)<sub>2</sub>)<sub>4</sub> (2b)). 2A crystallizes as a solvate in the triclinic space group P.hivin.1 (a 13.857(2), b 16.843(3), c 19.318(2) .ANG., .alpha. 79.23(2), .beta. 76.855(13), .gamma. 70.10(2).degree., Z = 2) and solvated 2b in the monoclinic space group P21 (a 12.710(3), b 23.251(3), c 18.702(4) .ANG., .beta. 101.16(2).degree., Z = 2). The cations contain a {Co<sub>3</sub>(OMe)<sub>4</sub>} cube fragment core with an .eta.3-Me<sub>3</sub>TAC bonded to each Co atom. Me<sub>3</sub>TAC is bonded unsym. due to H-bonding interactions with the anions. This broken symmetry can also be obsd. as solvent-, anion-, and H/D-isotope-dependent splitting of the signals in <sup>1</sup>H and <sup>2</sup>H NMR. A byproduct of the reaction is the protonated Me<sub>3</sub>TAC. The analogous monoacid adduct Me<sub>3</sub>TAC.cndot.HCl was characterized by x-ray crystallog. (orthorhombic space group Pbca, a 11.0366(9), b 12.2986(6), c 13.9949(7) .ANG., Z = 8).  
ST crystal structure cobalt trimethyltriazacyclohexane methoxo trinuclear; structure cobalt trimethyltriazacyclohexane methoxo partial cubane; cobalt trimethyltriazacyclohexane methoxo partial cubane prepn; azacyclohexane cobalt methoxo partial cubane prepn; hydrogen bond cobalt trimethyltriazacyclohexane methoxo trinuclear  
IT Bond length  
(cobalt-nitrogen; in cobalt trimethyltriazacyclohexane methoxo trinuclear partial cubane)

IT NMR (nuclear magnetic resonance)  
(of cobalt trimethyltriazacyclohexane methoxo partial cubane)  
IT Hydrogen bond  
(of cobalt trimethyltriazacyclohexane methoxo trinuclear partial  
cubane)  
IT Crystal structure  
Molecular structure  
(of trimethyltriazacyclohexane hydrochloride and its cobalt methoxo  
trinuclear partial cubane)  
IT Cluster compounds  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and crystal structure and hydrogen bonding of cobalt  
trimethyltriazacyclohexane methoxo partial cubane)  
IT 77-76-9, 2,2-Dimethoxypropane  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(for prepn. of cobalt trimethyltriazacyclohexane methoxo partial  
cubane)  
IT 198197-24-9P 198197-26-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(for prepn. of cobalt trimethyltriazacyclohexane methoxo partial  
cubane)  
IT 50-00-0, Formaldehyde, reactions 74-89-5, Methylamine, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(for prepn. of trimethyltriazacyclohexane)  
IT 198197-29-4P 198197-33-0P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and crystal structure and hydrogen bonding of)  
IT 198197-22-7P  
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(prepn. and crystal structure and reaction with cobalt aqua complex  
salts partial cubane)  
IT 198197-30-7P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and mol. structure and hydrogen bonding of)

L3 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS  
AN 1997:157895 CAPLUS  
TI Triazacyclohexane complexes of transition metals for olefin  
polymerization.  
AU Koehn, R. D.; Haufe, M.; Seifert, G.; Kociok-Koehn, G.  
CS Inst. f. Anorg. u. Analyt. Chemie, Technische Universitat Berlin, Berlin,  
D - 10623, Germany  
SO Book of Abstracts, 213th ACS National Meeting, San Francisco, April 13-17  
(1997), INOR-431 Publisher: American Chemical Society, Washington, D. C.  
CODEN: 64AOAA  
DT Conference; Meeting Abstract  
LA English  
AB In the search for ancillary ligands enforcing unusual coordination  
geometries in complexes with potential catalytic activity, we investigated  
the coordination chem. of N-substituted 1,3,5-triazacyclohexanes (R3TAC).  
X-ray crystallog. on several complexes has shown that this ligand  
coordinates facially to a variety of transition metals with N-M-N bite  
angles of around 60.degree. and severely misdirected nitrogen lone pairs  
deviating from the direct N-M bond by 25-45.degree.. [(R3TAC)CrCl<sub>3</sub>]  
reacts with {MeAlO}.chi. (MAO) to solns. that polymerize ethylene. As a  
model for the active species we attempted to prep. complexes  
[(R3TAC)MR]<sup>n+</sup>. As a first structural model, [(R3TAC)ZnEt]<sup>+</sup> was prep'd.  
from ZnEt<sub>2</sub> and R3TAC/PhNMe<sub>2</sub>H<sup>+</sup>. Several complexes (R3TAC)CrR'<sub>3</sub> were prep'd.  
However, we were unable to isolate the desired cationic Cr(III) complexes  
by protonolysis. Similar Cr(II) complexes were also investigated.

L3 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS  
AN 1996:584666 CAPLUS  
DN 125:276048  
TI The chemistry of 1,3,5-triazacyclohexane complexes. 5. Cationic zinc(II)

alkyl complexes of N-alkylated 1,3,5-triazacyclohexanes and  
 13-benzyl-1,5,9-triazatricyclo[7.3.1.05,13]tridecane  
**AU** Haufe, Matthias; Koehn, Randolph D.; Wiemann, Roman;  
 Seifert, Guido; Zeigan, Dieter  
**CS** Institut Fuer Anorganische und Analytische Chemie, Technische Universitaet  
 Berlin, Berlin, D-10623, Germany  
**SO** Journal of Organometallic Chemistry (1996), 520(1-2), 121-129  
 CODEN: JORCAI; ISSN: 0022-328X  
**PB** Elsevier  
**DT** Journal  
**LA** English  
**CC** 29-9 (Organometallic and Organometalloidal Compounds)  
 Section cross-reference(s): 75  
**GI**



- AB** Diethylzinc reacts with hydroperchlorates of N-alkylated 1,3,5-triazacyclohexanes ( $R_3TAC$ ;  $R = Me, PhCH_2, iPr$ ) and with the hydrotetrafluoroborate of 1,3,5-tris(*p*-fluorobenzyl)-1,3,5-triazacyclohexane ( $FBz_3TAC$ ) to give the corresponding cationic Zn complexes  $[(R_3TAC)Zn(Et)][X]$  ( $X = ClO_4^-, BF_4^-$ ), e.g., I. Similar complexes were obtained from diethylzinc treated with  $[HNMe_2Ph][BF_4]$  or  $[HNMe_2Ph][B(C_6F_5)_4](Et_2O)$  in the presence of  $R_4TAC$  ( $R = PhCH_2, p\text{-FC}_6H_4CH_2, S\text{-PhMeCH}$ ). The crystal structure of II, a product of the decomprn. of I, was detd. The structures of  $[(S\text{-PhMeCH})_3TAC]Zn(ET)][BF_4]$  and  $[(p\text{-FC}_6H_4CH_2)_3TAC]Zn(Et)][BF_4]$  were estd. using nuclear Overhauser enhancement spectroscopy. Protonolysis of diethylzinc with  $[HNMe_2Ph][BF_4]$  in the presence of 13-benzyl-1,5,9-triazatricyclo[7.3.1.05,13]tridecane ( $BzTATC$ ) yield  $[(BzTATC)Zn(Et)][BF_4]$ .  
**ST** crystal structure triazacyclohexenium; mol structure triazacyclohexenium; zinc triazacyclohexane triazatricyclotridecane complex prepn; NOESY triazacyclohexane zinc complex; mol mechanics triazacyclohexane zinc complex  
**IT** Crystal structure  
 Molecular structure  
 (of triazacyclohexenium)  
**IT** 51720-36-6P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and crystal structure of)  
**IT** 118612-00-3P 182175-58-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
**IT** 108-74-7 121-69-7, N,N-Dimethylaniline, reactions 557-20-0,  
 Diethylzinc 2547-66-2 4520-86-9 10556-98-6 131968-96-2  
 173449-39-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)

(prep. of cationic zinc(II) alkyl complexes of N-alkylated triazacyclohexanes and benzyltriazatricyclotridecane)  
IT 22533-76-2P 69737-15-1P 182175-60-6P 182175-65-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prep. of cationic zinc(II) alkyl complexes of N-alkylated triazacyclohexanes and benzyltriazatricyclotidecane)  
IT 182175-68-4P 182175-70-8P 182175-71-9P 182175-72-0P 182175-75-3P  
182175-77-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prep. of cationic zinc(II) alkyl complexes of N-alkylated triazacyclohexanes and benzyltriazatricyclotidecane)

L3 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS  
AN 1996:48776 CAPLUS  
DN 124:276702  
TI The chemistry of 1,3,5-triazacyclohexane complexes. Part 3. High yield synthesis of [Cr{N(SiMe<sub>3</sub>)<sub>2</sub>}<sub>3</sub>] and accurate structure determination by cocrystallization with Me<sub>6</sub>Si<sub>2</sub>  
AU Koehn, Randolph D.; Kociok-Koehn, Gabriele; Haufe, Matthias  
CS Inst. Anorg. Anal. Chem., Tech. Univ. Berlin, Berlin, D-10623, Germany  
SO Chemische Berichte (1996), 129(1), 25-7  
CODEN: CHBEAM; ISSN: 0009-2940  
PB VCH  
DT Journal  
LA English  
CC 78-5 (Inorganic Chemicals and Reactions)  
Section cross-reference(s): 75  
AB The reaction of the [CrLC<sub>13</sub>] (L = N,N',N''-trimethyl-1,3,5-triazacyclohexane) with LiN(SiMe<sub>3</sub>)<sub>2</sub> or NaN(SiMe<sub>3</sub>)<sub>2</sub> in petroleum ether yielded nearly quant. [Cr{N(SiMe<sub>3</sub>)<sub>2</sub>}<sub>3</sub>] (I) with loss of L. I was crystd. from Me<sub>6</sub>Si<sub>2</sub> as [Cr{N(SiMe<sub>3</sub>)<sub>2</sub>}<sub>3</sub>].cntdot.(Me<sub>6</sub>Si<sub>2</sub>)<sub>0.5</sub> which allowed the refinement of the x-ray crystal structure in the trigonal space group P31c (a 16.012, c 8.4796 .ANG., V = 1882.8 .ANG.<sub>3</sub>, Z = 2) without severe disorder.  
ST triazacyclohexane chromium complex reaction silylamine; chromium silylamine complex prepn; crystal structure chromium silylamine complex; mol structure chromium trimethylsilylamine complex  
IT Crystal structure  
Molecular structure  
(of chromium bis(trimethylsilyl)amide)  
IT 175285-80-OP  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(crystal structure; prepn. of bis(trimethylsilylamine) chromium from triazacyclohexane chromium and bis(trimethylsilylamine) lithium)  
IT 175285-79-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(des prepn. of bis(trimethylsilylamine) chromium from triazacyclohexanechromium and bis(trimethylsilylamine) lithium)  
IT 4039-32-1, Lithium Bis(trimethylsilyl)amide  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(prep. of bis(trimethylsilylamine) chromium from triazacyclohexane chromium and bis(trimethylsilylamine) lithium)

L3 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS  
AN 1995:847433 CAPLUS  
DN 124:56199  
TI .eta.-3-1,3,5-Triazacyclohexane complexes of tribenzylchromium(III)  
AU Koehn, Randolph D.; Kociok-Koehn, Gabriele; Haufe, Matthias  
CS Institut fuer Anorganische und Analytische Chemie, Technische Universitaet Berlin, Strasse des 17, Juni 135, Berlin, D-10623, Germany  
SO Journal of Organometallic Chemistry (1995), 501(1-2), 303-7  
CODEN: JORCAI; ISSN: 0022-328X  
PB Elsevier  
DT Journal

LA English  
CC 29-11 (Organometallic and Organometalloidal Compounds)  
Section cross-reference(s): 75  
AB 1,3,5-Tribenzyl-1,3,5-triazacyclohexane ('Bz3TAC') and  
1,3,5-tricyclohexyl-1,3,5-triazacyclohexane ('Cy3TAC') react with  
CrCl<sub>3</sub>(THF)<sub>3</sub> to the corresponding complexes (Bz3TAC)CrCl<sub>3</sub> (1a) and  
(Cy3TAC)CrCl<sub>3</sub> (1b). These react with benzylsodium in toluene to the  
tribenzylchromium(III) complexes (Bz3TAC)Cr(CH<sub>2</sub>Ph)<sub>3</sub> (2a) and  
(Cy3TAC)Cr(CH<sub>2</sub>Ph)<sub>3</sub> (2b). The crystal and mol. structure of  
2b.cndot.1.5toluene was detd. by x-ray diffraction.  
ST crystal structure chromium benzyl triazacyclohexane complex; mol structure  
chromium benzyl triazacyclohexane complex  
IT Crystal structure  
Molecular structure  
(of chromium benzyl triazacyclohexane complex)  
IT Crystal field theory and Ligand field theory  
(of chromium triazacyclohexane complexes)  
IT Energy level splitting  
(crystal-field, of chromium triazacyclohexane complexes)  
IT 1121-53-5, Benzylsodium  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(for prepn. of chromium benzyl triazacyclohexane complexes)  
IT 2547-66-2, 1,3,5-Tribenzyl-1,3,5-triazacyclohexane  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(for prepn. of chromium complexes)  
IT 6281-14-7P, 1,3,5-Tricyclohexyl-1,3,5-triazacyclohexane  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(for prepn. of chromium complexes)  
IT 10170-68-0, Trichlorotris(tetrahydrofuran)chromium  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(for prepn. of triazacyclohexane complexes)  
IT 108-91-8, Cyclohexylamine, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(for prepn. of tricyclohexyltriazacyclohexane)  
IT 172166-81-3P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and crystal structure of)  
IT 172166-84-6P, Tris(benzyl)(1,3,5-tribenzyl-1,3,5-  
triazacyclohexane)chromium  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and ligand-field parameters)  
IT 172166-82-4P, Trichloro(1,3,5-tribenzyl-1,3,5-triazacyclohexane)chromium  
172166-83-5P, Trichloro(1,3,5-tricyclohexyl-1,3,5-  
triazacyclohexane)chromium  
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(prepn., ligand-field parameters and reaction with benzylsodium)  
IT 172166-80-2P, Tris(benzyl)(1,3,5-tricyclohexyl-1,3,5-  
triazacyclohexane)chromium  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(prepn., mol. structure and ligand-field parameters)

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